

Supporting Information

Nonlinear Absorbing Cationic Iridium(III) Complexes Bearing Benzothiazolylfluorene Motif on the Bipyridine (N[^]N) Ligand: Synthesis, Photophysics and Reverse Saturable Absorption

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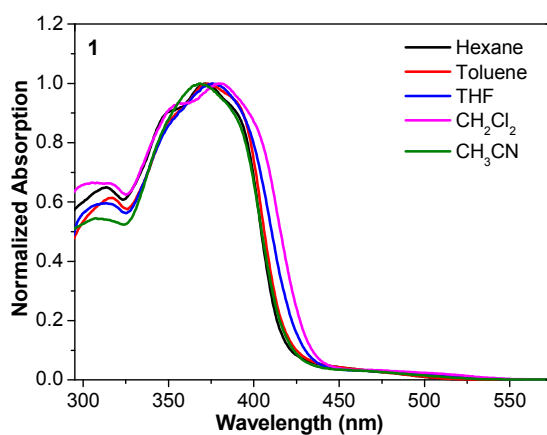


Figure S1. Normalized UV-vis absorption spectra of **1** in different solvents.

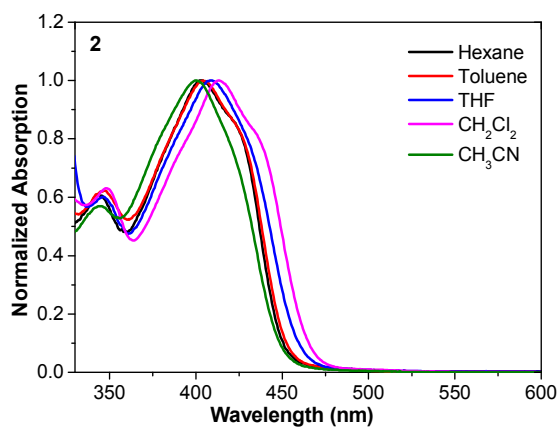


Figure S2. Normalized UV-vis absorption spectra of **2** in different solvents.

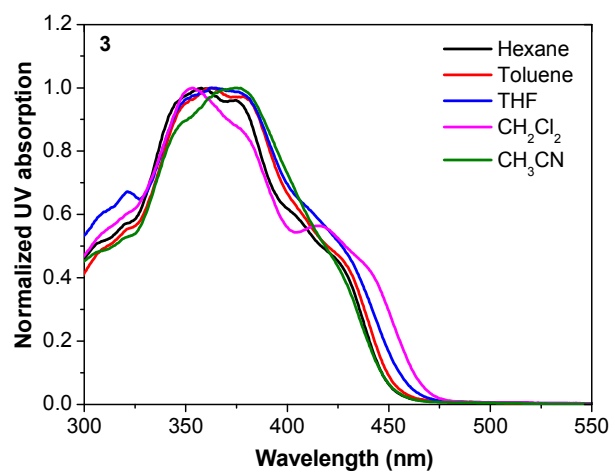


Figure S3. Normalized UV-vis absorption spectra of **3** in different solvents.

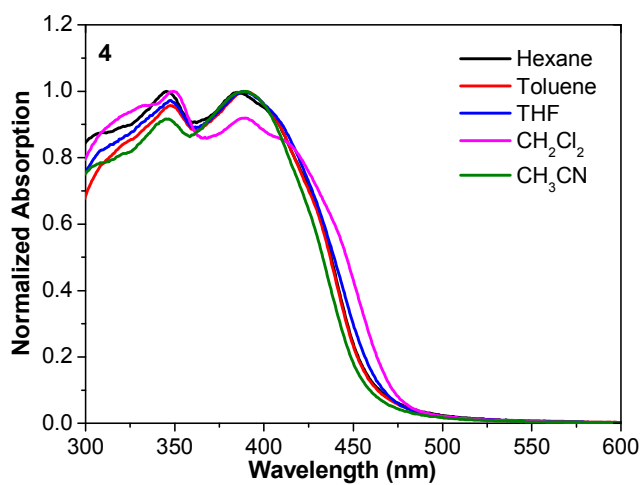


Figure S4. Normalized UV-vis absorption spectra of **4** in different solvents.

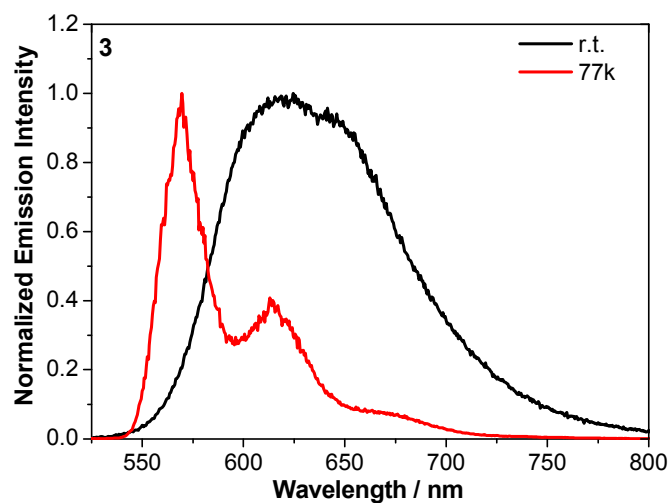


Figure S5. Normalized emission spectra of complex **3** ($\lambda_{\text{ex}} = 418$ nm) at r.t. and 77 K in BuCN.

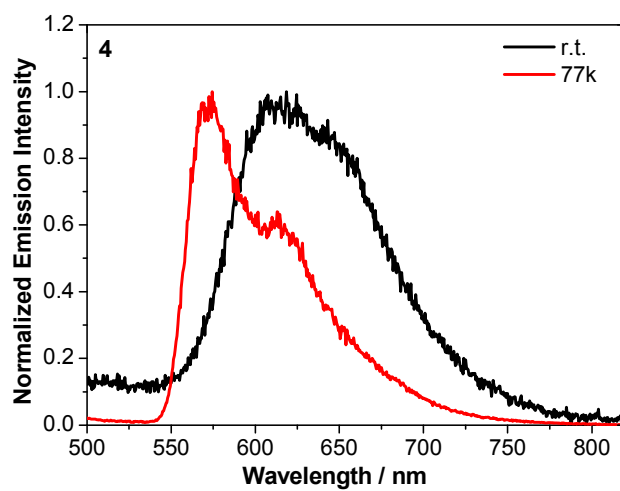


Figure S6. Normalized emission spectra of complex **4** ($\lambda_{\text{ex}} = 420$ nm) at r.t. and 77 K in BuCN.

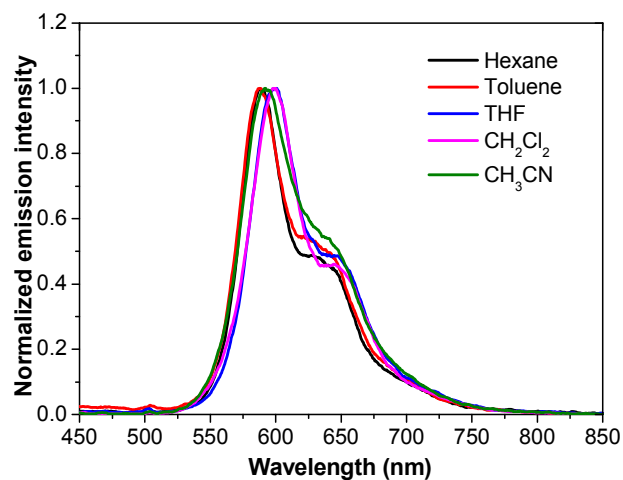


Figure S7. Normalized emission spectra of **2** in different degassed solvents ($\lambda_{\text{ex}} = 436$ nm).

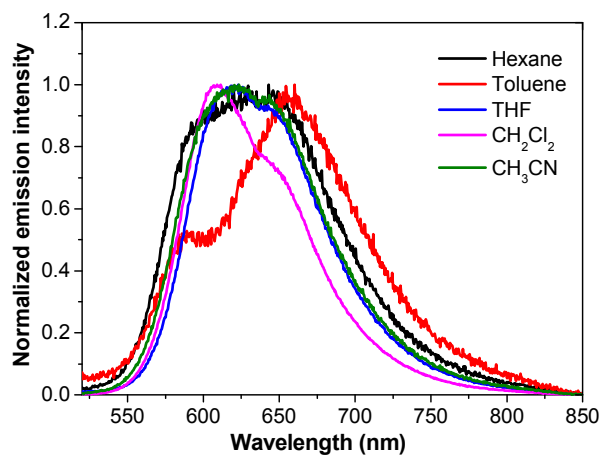


Figure S8. Normalized emission spectra of **3** in different degassed solvents ($\lambda_{\text{ex}} = 436$ nm).

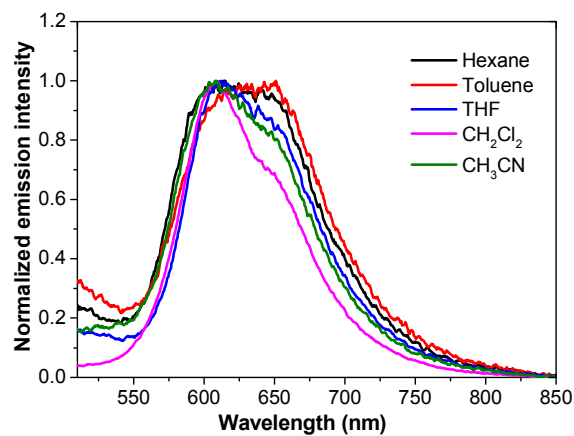


Figure S9. Normalized emission spectra of **4** in different degassed solvents ($\lambda_{\text{ex}} = 436$ nm).

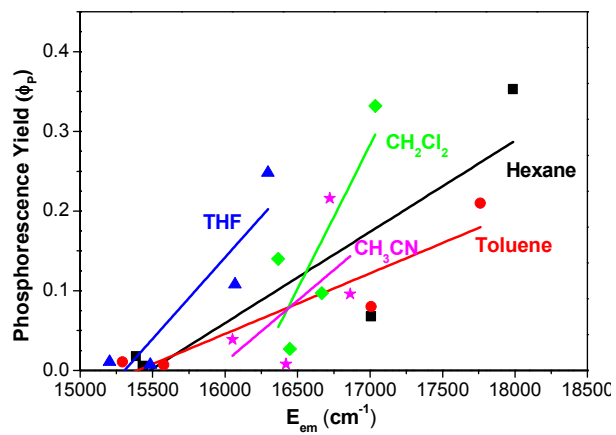


Figure S10. Correlation diagram for the emission quantum yield (Φ_{em}) vs. emission energy (E_{em}) in different solvents for **1-4**.

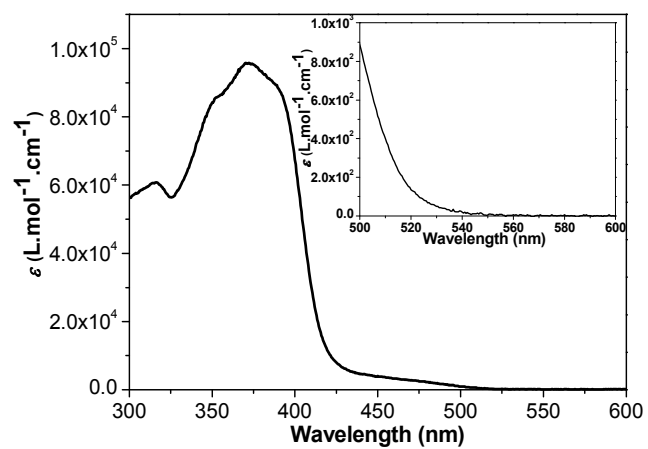


Figure S11. UV-vis absorption spectrum of **1** in toluene.

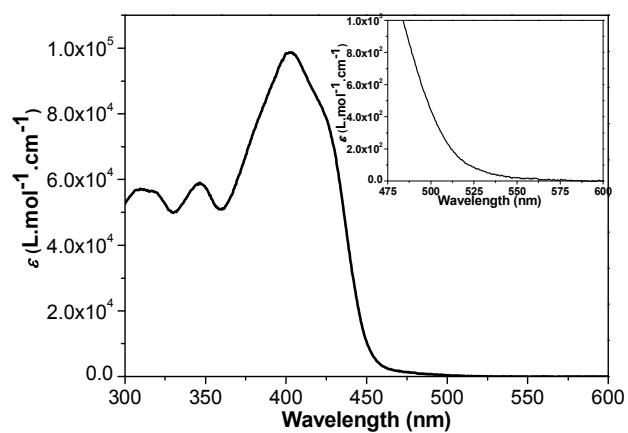


Figure S12. UV-vis absorption spectrum of **2** in toluene.

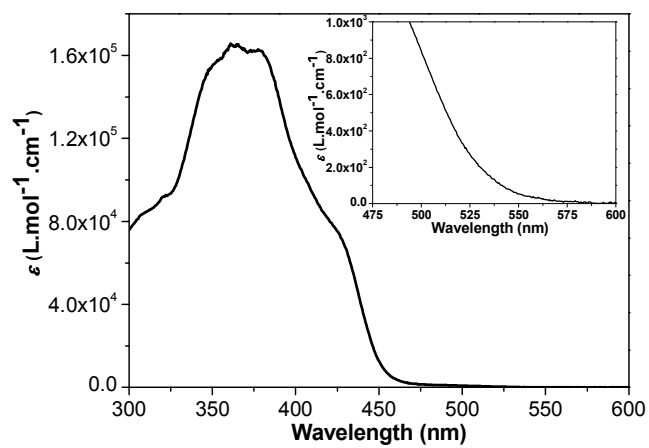


Figure S13. UV-vis absorption spectrum of **3** in toluene.

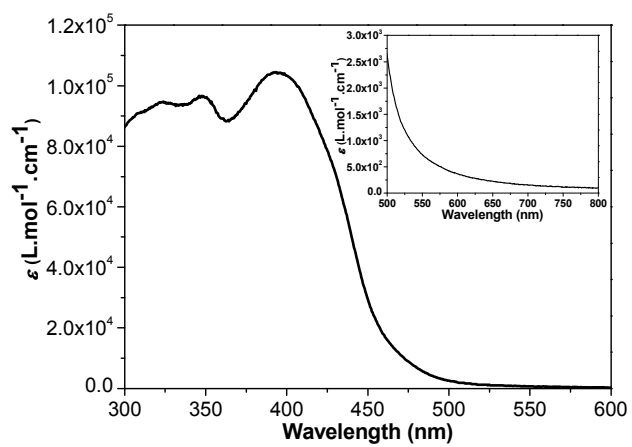
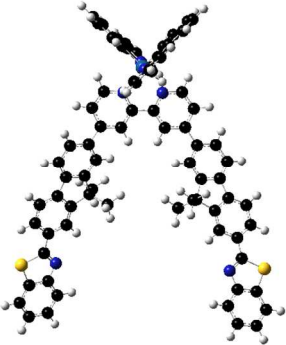
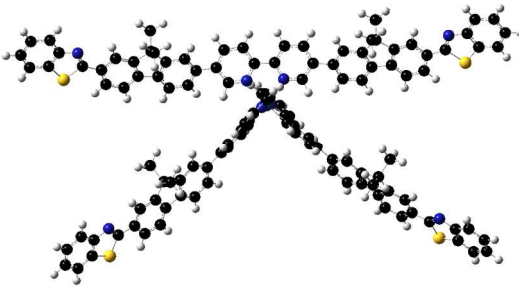
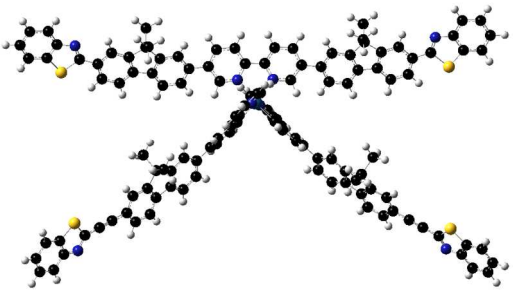


Figure S14. UV-vis absorption spectrum of **4** in toluene.

Table S1. Optimized geometries for complexes **1-4** in CH₂Cl₂ using PBE1 functional and LANL2DZ basis set

Complex	Optimized Geometry
1	
2	
3	
4	

Reference

(57) Frisch, M. J. T. G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, Jr., J. A.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, N. J.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, Ö.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. Gaussian 09; Revision A.1, ed.; Gaussian, Inc., Wallingford CT, 2009.